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# ADIABATIC PHASE BOUNDARY PROPAGATION IN A THERMOELASTIC SOLID

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# Adiabatic Phase Boundary Propagation in a Thermoelastic Solid.

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#### Abstract

The dynamical aspects of solid-solid phase transformations are studied within the framework of the theory of thermoelasticity. A problem of the Riemann type for a one-dimensional bar undergoing an adiabatic process is analyzed. It is shown that by imposing a kinetic relation and a nucleation criterion it is possible to single out a unique solution. This extends to the thermomechanical case results previously found in a purely mechanical context.

### 1 Introduction.

Solid-solid phase transitions can occur in materials by a change in stress or temperature. At a macroscopic level, within the framework of thermo-elasticity, materials that exist in different solid phases can be modeled by a nonconvex Helmholtz free energy density that depends smoothly on the deformation gradient and the temperature. At some fixed temperature, the Helmholtz potential exhibits multiple wells as a function of the deformation gradient. Each well is associated to a distinct solid phase.

In a one-dimensional setting, ABEYARATNE & KNOWLES [4] analyzed an initial value problem of the Riemann type for a bar made of a special thermoelastic material that can sustain multiple phases. It was found that the solution to the *adiabatic* Riemann problem, which involves initial data from two *distinct* phases, is *not* unique. Because of the nonconvexity of the the Helmholtz potential, the structure of the solution involves two types of discontinuities, viz., *shock waves* and *phase boundaries* (see, e.g., ABEYARATNE & KNOWLES [1]-[4], SHEARER [7], SLEMROD [8], TRUSKINOVSKY [10]). The solution can be determined *up to* the phase boundary velocity.

Based on the formalism of non-equilibrium thermodynamics (see, e.g., Callen [5], Truesdell [9]) and classical concepts used in materials science (see, e.g., Christian [6]), Abeyaratne & Knowles propose the existence of an additional piece of constitutive information, a *kinetic relation*, which applies at subsonic phase boundaries. The kinetic relation relates the phase boundary velocity to the *driving traction*, which is associated to a jump in entropy across the phase boundary. With this additional relation, it is possible to single out a unique solution for the Riemann problem (see Abeyaratne

#### & Knowles [1]-[4]).

The purpose of the present analysis is to investigate, within the context of the adiabatic theory, the Riemann problem involving initial data from the same phase. The results are qualitatively different from those in [4] in the sense that, in order to recover uniqueness, a nucleation criterion has to be enforced. This nucleation criterion signals the onset of a phase change and generalizes, for the thermoelastic case, the results found in [3] in the context of a purely mechanical theory.

In Section 2, the governing field equations and the corresponding jump conditions for an adiabatic process are obtained from balance principles. A particular thermoelastic material is introduced in Section 3. The field equation and jump conditions are specialized for this material in Section 4. An initial value problem of the Riemann type for a one-dimensional bar is formulated in Section 5. It is found that there exist two different kinds of solutions. One kind involves no phase transition, whereas the other kind involves a twoparameter family of solutions containing two propagating phase boundaries (the phase boundary velocities acting as parameters). In the latter case, a kinetic relation is used to obtain the phase boundary velocities and hence the solution is fully determined. It is also found that for some range of the initial data, it is possible to have either kind of solution (i.e., with or without phase boundaries). Therefore, a nucleation criterion is enforced to single out the unique solution to the problem from the two different kinds. Finally, in Section 7, the connection between the Riemann problem with uniform data and the nucleation criterion is investigated.

#### 2 Preliminaries.

Consider longitudinal motions of a bar with uniform cross section that occupies the interval [-L, L] in an unstressed reference configuration during a time interval  $[t_0, t_1]$ . Assume that the referential mass density  $\rho$  is uniform. Let  $(x,t) \in [-L, L] \times [t_0, t_1]$  be a point in the reference configuration that is mapped to the position y(x,t) = x + u(x,t), where u is the displacement. It is assumed that  $u \in C^0([-L, L] \times [t_0, t_1])$  and piecewise  $C^2([-L, L] \times [t_0, t_1])$ . Let  $\gamma = u_x$  and  $v = u_t$  be the strain and particle velocity respectively (the subscript refers to partial differentiation). The restriction  $-1 < \gamma(x,t)$ ,  $\forall x,t$ , guarantees that the deformation  $y(\cdot,t)$  is invertible at each t. Let  $\sigma$  be the stress,  $\epsilon$  the internal energy per unit referential mass and  $\eta$  the entropy per unit referential mass. Assume that  $\sigma$ ,  $\epsilon$  and  $\eta$  are piecewise  $C^1([-L, L] \times [t_0, t_1])$ . The balance of linear momentum, balance of energy and the Clausius-Duhem inequality (dissipation inequality) for an adiabatic thermomechanical process in a one-dimensional bar are

$$[\sigma]_{x_1}^{x_2} = \frac{d}{dt} \int_{x_1}^{x_2} \rho v dx , \qquad (1)$$

$$[\sigma v]_{x_1}^{x_2} = \frac{d}{dt} \int_{x_1}^{x_2} \rho\left(\epsilon + \frac{1}{2}v^2\right) dx , \qquad (2)$$

$$\Gamma(t) = \frac{d}{dt} \int_{x_1}^{x_2} \rho \eta dx \ge 0 , \qquad (3)$$

 $\forall t \in [t_0, t_1] \text{ and } \forall [x_1, x_2] \subseteq [-L, L].$  Here,  $\Gamma(t)$  is the entropy production rate in the interval  $[x_1, x_2]$ . Localization of the balance laws (1)-(3) at points

where the fields are smooth provides

$$\sigma_x = \rho v_t \ , \tag{4}$$

$$(\sigma v)_x = \rho \left(\epsilon + \frac{1}{2}v^2\right)_{\star} , \qquad (5)$$

$$\eta_t \ge 0 \ . \tag{6}$$

The compatibility equation is

$$v_x = \gamma_t \ . \tag{7}$$

Equation (5), with the use of (4), can be expressed as

$$\sigma \gamma_t = \rho \epsilon_t \ . \tag{8}$$

Suppose that there is a point x = s(t) in  $[x_1, x_2]$  at which some (or all) fields are discontinuous. Localization at x = s(t) of the global balances (1)-(3) and the compatibility equation (7) provide the corresponding jump conditions, viz.,

$$\llbracket v \rrbracket + \dot{s} \llbracket \gamma \rrbracket = 0 , \qquad (9)$$

$$\llbracket \sigma \rrbracket + \rho \dot{s} \llbracket v \rrbracket = 0 , \qquad (10)$$

$$[\![\sigma v]\!] + \rho \dot{s} [\![\epsilon + \frac{1}{2}v^2]\!] = 0 ,$$
 (11)

$$\llbracket \eta \rrbracket \dot{s} \le 0 , \qquad (12)$$

where  $\dot{s} = ds/dt$  is the speed of propagation of the discontinuity and, for any function g,

$$[g] \equiv g^+ - g^-, \quad g^- = \lim_{x \to s(t)^-} g(x, t), \quad g^+ = \lim_{x \to s(t)^+} g(x, t).$$

Discontinuities are classified into two types, viz., classical shock waves and phase boundaries. Shock waves are related to discontinuities where the material on each side is in the same phase, whereas phase boundaries refer to discontinuities where different material phases exist on each side. In the adiabatic theory, a shock wave whose Lagrangian velocity  $\dot{s}$  is zero is referred to as a contact discontinuity (i.e., the material particles on each side of the discontinuity are the same at all times). Specific jump conditions in each case are given in Section 4.

Let the Helmholtz potential be given by  $\psi = \bar{\psi}(\gamma, \theta)$ . This potential is related to the internal energy through

$$\psi = \epsilon - \theta \eta \ . \tag{13}$$

For a classical thermoelastic material, the stress  $\sigma$  and the entropy  $\eta$  are given by

$$\sigma = \bar{\sigma}(\gamma, \theta) = \rho \bar{\psi}_{\gamma}(\gamma, \theta) , \qquad (14)$$

$$\eta = \bar{\eta}(\gamma, \theta) = -\bar{\psi}_{\theta}(\gamma, \theta) . \tag{15}$$

The isothermal elastic modulus  $\mu$ , the specific heat at constant strain c and

the coefficient of thermal expansion  $\alpha$  are defined by

$$\mu = \bar{\mu}(\gamma, \theta) = \bar{\sigma}_{\gamma}(\gamma, \theta) = \rho \bar{\psi}_{\gamma\gamma}(\gamma, \theta) ,$$

$$c = \bar{c}(\gamma, \theta) = \theta \bar{\eta}_{\theta}(\gamma, \theta) = -\theta \bar{\psi}_{\theta\theta}(\gamma, \theta) ,$$

$$\alpha = \bar{\alpha}(\gamma, \theta) = -\frac{\bar{\sigma}_{\theta}(\gamma, \theta)}{\bar{\sigma}_{\gamma}(\gamma, \theta)} = -\frac{\bar{\psi}_{\gamma\theta}(\gamma, \theta)}{\bar{\psi}_{\gamma\gamma}(\gamma, \theta)} .$$

$$(16)$$

The isothermal sound speed is defined, when  $\mu > 0$ , as

$$a = \bar{a}(\gamma, \theta) = \sqrt{\frac{\bar{\mu}(\gamma, \theta)}{\rho}}$$
 (17)

Proper phase boundaries travel at *subsonic* velocities (see also Truski-Novsky [10]). Using equations (13), (14) and (15) in equation (8) provides an alternative expression for the energy equation, i.e.,

$$\eta_t = 0 \ . \tag{18}$$

It follows that the dissipation inequality (6) is trivially satisfied at regular points. The rate of entropy production for a segment  $[x_1, x_2]$  of the bar which contains a propagating discontinuity at x = s(t) can be expressed as

$$\Gamma(t) = \Gamma_b(t) + \Gamma_s(t) , \qquad (19)$$

where

$$\Gamma_b(t) = \int_{x_1}^{x_2} \rho \eta_t dx , \qquad (20)$$

$$\Gamma_s(t) = -\rho \llbracket \eta \rrbracket \dot{s} \ . \tag{21}$$

Here,  $\Gamma_b$  represents the bulk entropy production and  $\Gamma_s$  corresponds to the entropy production due to the moving discontinuity. Equations (18) and (20) imply that

$$\Gamma_b = 0 , \qquad (22)$$

hence the entropy production for a thermoelastic material under an adiabatic process occurs solely because of the presence of a moving discontinuity. Based on this entropy production, define the *driving traction* as

$$f = -\rho \llbracket \eta \rrbracket \langle \theta \rangle \ . \tag{23}$$

For a discussion of the notion of driving traction, see ABEYARATNE & KNOWLES [1] and TRUSKINOVSKY [10]. The velocity jump can be eliminated from (11) by using equations (9) and (10), i.e.,

$$(\rho \llbracket \epsilon \rrbracket - \langle \sigma \rangle \llbracket \gamma \rrbracket) \dot{s} = 0 , \qquad (24)$$

where, for any function g,

$$\langle g \rangle \equiv \frac{1}{2} \left( g^+ + g^- \right) .$$

From the energy jump condition (24), when  $\dot{s} \neq 0$ , it follows that

$$\rho[\![\epsilon]\!] = \langle \sigma \rangle[\![\gamma]\!] \ .$$

Moreover, since  $\llbracket \eta \theta \rrbracket = \langle \eta \rangle \llbracket \theta \rrbracket + \llbracket \eta \rrbracket \langle \theta \rangle$ , then (13), (23) and the above relation

provide the following equivalent expression for the driving traction:

$$f = \rho \llbracket \psi \rrbracket - \langle \sigma \rangle \llbracket \gamma \rrbracket + \rho \langle \eta \rangle \llbracket \theta \rrbracket . \tag{25}$$

For a thermoelastic material, (14), (15) and (25) give

$$f = \rho \left\{ \llbracket \psi \rrbracket - \langle \psi_{\gamma} \rangle \llbracket \gamma \rrbracket - \langle \psi_{\theta} \rangle \llbracket \theta \rrbracket \right\} . \tag{26}$$

In terms of the driving traction, the dissipation inequality (12) can be expressed as

$$f\dot{s} \ge 0. \tag{27}$$

The driving traction plays an important role in the kinetic relation and the nucleation criterion as explained in Section 6.

### 3 Thermoelastic material.

ABEYARATNE & KNOWLES [2] proposed an analytical model of a thermoelastic material that can exist in different solid phases. The model is simple yet it incorporates the fundamental characteristics of a phase-changing material and allows to obtain results in specific problems. A phase diagram of this material in the  $\gamma$ , $\theta$ -plane is shown in Figure 1. For temperatures below a *crit*ical temperature  $\theta_C$ , the material can exist in either a low strain phase  $P_1$  or a high strain phase  $P_3$ . These phases are thermodynamically metastable and are separated by an unstable phase  $P_2$ . Above the critical temperature the material can only exist in a stable phase P. Throughout this analysis, only transformations from or to the low and high strain phases are considered. Moreover, for a fixed temperature below the transformation temperature  $\theta_T$ , the absolute minimum of the Helmholtz potential corresponds to the high strain phase and for a fixed temperature between the transformation temperature and the critical temperature, the absolute minimum corresponds to the low strain phase. A thorough description of the thermomechanical characteristics of this material can be found in [2]. The boundaries between the different phases are given by

$$\gamma_M(\theta) = \gamma_C + M(\theta - \theta_C) , 
\gamma_m(\theta) = \gamma_C + m(\theta - \theta_C) ,$$
(28)

where  $\gamma_C > 0$ ,  $\theta_C > 0$ , M and m are constants. The expression for the Helmholtz potential is given in each phase by

$$\bar{\psi}(\gamma,\theta) = \begin{cases}
\frac{\mu}{2\rho} \gamma^2 - \frac{\alpha\mu}{\rho} \gamma(\theta - \theta_T) - c\theta \log\left(\frac{\theta}{\theta_T}\right) & \text{in } P_1, \\
\frac{\mu}{2\rho} (\gamma - \gamma_T)^2 - \frac{\alpha\mu}{\rho} (\gamma - \gamma_T)(\theta - \theta_T) & \\
-c\theta \log\left(\frac{\theta}{\theta_T}\right) + \frac{\lambda_T}{\theta_T} (\theta - \theta_T) & \text{in } P_3,
\end{cases}$$
(29)

where  $\gamma_T$  is the transformation strain and  $\lambda_T$  is the latent heat at the transformation temperature. The remaining parameters were defined in Section 3 and are assumed constant. The expression in the unstable phase  $P_2$  is not relevant here. According to the model developed in [2], the material parameters

must satisfy the following restrictions:

$$\gamma_T > (M - m)\theta_C > 0 ,$$

$$\gamma_C = \frac{\gamma_T}{2} + \frac{1}{2}(M + m)(\theta_C - \theta_T) ,$$

$$M + m = \frac{2\rho\lambda_T}{\mu\gamma_T\theta_T} + 2\alpha .$$
(30)

The first restriction guarantees that there is no overlap between the two metastable phases in the  $\gamma$ , $\theta$ -plane (hence, the stress is uniquely determined for a given temperature and strain). Restrictions (30)<sub>2,3</sub> are related to the fact that the metastable phases and the unstable phase coincide at the critical point ( $\gamma_C$ ,  $\theta_C$ ). From (14) and (29), the stress response function is given by

$$\bar{\sigma}(\gamma, \theta) = \begin{cases} \mu \gamma - \alpha \mu (\theta - \theta_T) & \text{in } P_1, \\ \\ \mu (\gamma - \gamma_T) - \alpha \mu (\theta - \theta_T) & \text{in } P_3. \end{cases}$$
(31)

Observe that, for a fixed temperature, the stress-strain relation is linear in each phase. Hence, this material will be referred to as the *trilinear* material. The entropy response function, from (15) and (29), is given by

$$\bar{\eta}(\gamma, \theta) = \begin{cases} \frac{\alpha \mu}{\rho} \gamma + c \log\left(\frac{\theta}{\theta_T}\right) + c & \text{in } P_1, \\ \frac{\alpha \mu}{\rho} (\gamma - \gamma_T) + c \log\left(\frac{\theta}{\theta_T}\right) + c - \frac{\lambda_T}{\theta_T} & \text{in } P_3. \end{cases}$$
(32)

It is convenient to introduce a set of nondimensional parameters for the trilinear material. Define the following parameters:

$$T = \frac{c\theta}{a^2 \gamma_T^2}, \quad \delta = \frac{\gamma}{\gamma_T}, \quad \bar{v} = \frac{v}{a \gamma_T},$$

$$v = \frac{\dot{s}}{a}, \quad M = \frac{a^2 \gamma_T M}{c}, \quad m = \frac{a^2 \gamma_T m}{c}, \quad l_T = \frac{\lambda_T}{a^2 \gamma_T^2}.$$
(33)

The variable  $\delta$  might be viewed as a "normalized" strain.

## 4 Field equations and jump conditions.

Henceforth, for simplicity, the coefficient of thermal expansion is taken as zero. Consequently, the mechanical and thermal effects are decoupled in the differential equations. Nevertheless, a connection between the strain and the temperature remains in place via the jump conditions. For the thermoelastic material introduced in Section 3, at points where the fields are smooth, (4), (7) and (8) provide, with  $\alpha = 0$ ,

$$\gamma_t - v_x = 0 (34)$$

$$v_t - a^2 \gamma_x = 0 , \qquad (35)$$

$$\theta_t = 0. (36)$$

The stress-strain relation, with  $\alpha = 0$ , is shown in Figure 2. The jump conditions (9)-(12) at a point of discontinuity where both sides are on the same phase, when  $\alpha = 0$  and using the nondimensional quantities (33), are

given by

$$[\![\delta]\!]\mathbf{v} + [\![\bar{v}]\!] = 0 ,$$

$$[\![\delta]\!] + [\![\bar{v}]\!]\mathbf{v} = 0 ,$$

$$[\![T]\!]\mathbf{v} = 0 ,$$

$$\log\left(\frac{T^{+}}{T^{-}}\right)\mathbf{v} \le 0 .$$

$$(37)$$

These jump conditions are equivalent to either

$$\begin{cases} v = \pm 1, \\ v[\![\delta]\!] + [\![\bar{v}]\!] = 0, \\ [\![T]\!] = 0, \end{cases} \text{ or } \begin{cases} v = 0, \\ [\![\delta]\!] = 0, \\ [\![\bar{v}]\!] = 0. \end{cases}$$
 (38)

The first case corresponds to a *shock wave* whereas the second is a *contact discontinuity*. Contact discontinuities are *stationary* in the reference configuration (i.e., in the Lagrangian sense). If the high strain phase is on the *right* of the phase boundary, then the jump conditions (9)-(12), when  $\alpha = 0$  and in nondimensional form, are given by

$$\mathbf{v}\llbracket\delta\rrbracket + \llbracket\bar{v}\rrbracket = 0 ,$$

$$\llbracket\delta\rrbracket - 1 + \mathbf{v}\llbracket\bar{v}\rrbracket = 0 ,$$

$$\left\{\llbracketT\rrbracket - \left(\langle\delta\rangle - \frac{1}{2}\right) - l_T\right\} \mathbf{v} = 0 ,$$

$$\left\{\log\frac{T^+}{T^-} - \frac{l_T}{T_T}\right\} \mathbf{v} \le 0 .$$

$$(39)$$

If the high strain phase is on the *left* of the phase boundary, then the jump conditions (9)-(12) are given by

$$\mathbf{v}\llbracket \delta \rrbracket + \llbracket \bar{v} \rrbracket = 0 ,$$

$$\llbracket \delta \rrbracket + 1 + \mathbf{v} \llbracket \bar{v} \rrbracket = 0 ,$$

$$\left\{ \llbracket T \rrbracket + \left( \langle \gamma \rangle - \frac{1}{2} \right) + l_T \right\} \mathbf{v} = 0 ,$$

$$- \left\{ \log \frac{T^-}{T^+} - \frac{l_T}{T_T} \right\} \mathbf{v} \le 0 .$$

$$(40)$$

## 5 Riemann problem.

Consider the Riemann problem corresponding to an infinitely long bar composed of the thermoelastic material described in Section 3. This problem can be formulated as follows: Find functions  $\delta(x,t)$ ,  $\bar{v}(x,t)$  and T(x,t) such that equations (34)-(36) are satisfied at points where the functions are sufficiently smooth and the corresponding jump conditions (38)-(40) are satisfied at points where the functions are discontinuous, subject to the following initial conditions:

$$\delta(x,0) , \bar{v}(x,0) , T(x,0) = \begin{cases} \delta_L , \bar{v}_L , T_L & \text{for } -\infty < x < 0 , \\ \delta_R , \bar{v}_R , T_R & \text{for } 0 < x < \infty . \end{cases}$$
(41)

It is assumed that, initially, the bar is in the low strain phase, in which case

$$\delta_L \in (-1, \delta_{\mathsf{M}}(T_L)] ,$$
  
 $\delta_R \in (-1, \delta_{\mathsf{M}}(T_R)] .$ 

The structure of the solution, as shown by ABEYARATNE & KNOWLES [4], must necessarily involve either *no* phase boundaries (in which case all particles of the bar remain in the original phase at all times) or *two* phase boundaries moving in opposite directions (in which case the particles jump to the high strain phase). In the latter case, as shown below, there is a two-parameter family of solutions.

#### 5.1 Solution with no phase boundary.

The solution with no phase boundary involves two shock waves (traveling along  $x/at = \pm 1$ ) and a contact discontinuity at x = 0. The bar remains in the low strain phase at all times. One seeks a self-similar solution of the form

$$\delta(x,t) , \bar{v}(x,t) , T(x,t) = \begin{cases} \delta_L , \bar{v}_L , T_L & \text{for } -\infty < x < -at , \\ \delta_0 , \bar{v}_0 , T_L & \text{for } -at < x < 0 , \\ \delta_0 , \bar{v}_0 , T_R & \text{for } 0 < x < at , \\ \delta_R , \bar{v}_R , T_R & \text{for } at < x < \infty , \end{cases}$$
(42)

where  $\delta_0$ ,  $\bar{v}_0$  are the only unknowns. Notice that the continuity of T across the shock waves and the continuity of  $\delta$  and  $\bar{v}$  across the contact discontinuity

were enforced. The solution is shown in Figure 3. Let

$$h = \frac{\delta_R + \delta_L}{2} + \frac{\bar{v}_R - \bar{v}_L}{2} \tag{43}$$

and

$$j = \frac{\delta_R - \delta_L}{2} + \frac{\bar{v}_R + \bar{v}_L}{2} ;$$

then, from the jump condition (38) it follows that

$$\delta_0 = h , \qquad (44)$$

$$\bar{v}_0 = j .$$

It was assumed that the bar was initially in the low strain phase, then, for the whole bar to remain in the low strain phase at all times and from (42), it is required that  $-1 < \delta_0 < \min \left[ \delta_{\mathsf{M}}(T_L), \delta_{\mathsf{M}}(T_R) \right]$ . Hence, from (44), there is a solution of the form (42) to the Riemann problem if and only if the initial datum h is such that

$$-1 < h \le \min\left[\delta_{\mathsf{M}}(T_L), \delta_{\mathsf{M}}(T_R)\right] . \tag{45}$$

### 5.2 Solutions with two phase boundaries.

The solution with two phase boundaries involves two shock waves (traveling along  $x/at = \pm 1$ ), a contact discontinuity at x = 0 and two phase boundaries at x/at = v < 0 and  $x/at = v_* > 0$ . One seeks a self-similar solution of the

form

$$\delta(x,t) , \ \bar{v}(x,t) , \ T(x,t) \ = \begin{cases} \delta_L , \bar{v}_L , T_L & \text{for } -\infty < x < -at \ , \\ \delta_0 , \bar{v}_0 , T_L & \text{for } -at < x < avt \ , \\ \delta_1 , \bar{v}_1 , T' & \text{for } avt < x < 0 \ , \\ \delta_1 , \bar{v}_1 , T'' & \text{for } 0 < x < av_*t \ , \\ \delta_2 , \bar{v}_2 , T_R & \text{for } av_*t < x < at \ , \\ \delta_R , \bar{v}_R , T_R & \text{for } at < x < \infty \ , \end{cases}$$

$$(46)$$

where  $\delta_0$ ,  $\delta_1$ ,  $\delta_2$ ,  $\bar{v}_0$ ,  $\bar{v}_1$ ,  $\bar{v}_2$ , T' and T'' are unknown. Notice that the continuity of T across the shock waves and the continuity of T across the contact discontinuity were enforced. Here, as in the previous section, the bar is initially in the low strain phase. The form of the solution is shown in Figure 4. From the jump conditions (38), (39)<sub>1,2</sub> and (40)<sub>1,2</sub>, one has

$$\begin{split} -(\delta_0 - \delta_L) + (\bar{v}_0 - \bar{v}_L) &= 0 \ , \\ \mathbf{v}(\delta_1 - \delta_0) + (\bar{v}_1 - \bar{v}_0) &= 0 \ , \\ \mathbf{v}_*(\delta_2 - \delta_1) + (\bar{v}_2 - \bar{v}_1) &= 0 \ , \\ (\delta_R - \delta_2) + (\bar{v}_R - \bar{v}_2) &= 0 \ , \\ (\delta_1 - \delta_0 - 1) + (\bar{v}_1 - \bar{v}_0) \mathbf{v} &= 0 \ , \\ (\delta_2 - \delta_1 + 1) + (\bar{v}_2 - \bar{v}_1) \mathbf{v}_* &= 0 \ . \end{split}$$

Solving this system provides

$$\delta_{0} = h + \frac{1}{2} \left( \frac{1}{1 + v_{*}} - \frac{1}{1 + v} \right) ,$$

$$\delta_{1} = h + \frac{1}{2} \left( \frac{1}{1 - v} + \frac{1}{1 + v_{*}} \right) ,$$

$$\delta_{2} = h + \frac{1}{2} \left( \frac{1}{1 - v} - \frac{1}{1 - v_{*}} \right) ,$$

$$(47)$$

and

$$\bar{v}_{0} = j + \frac{1}{2} \left( \frac{1}{1 + v_{*}} - \frac{1}{1 + v} \right) ,$$

$$\bar{v}_{1} = j + \frac{1}{2} \left( \frac{1}{1 + v_{*}} - \frac{1}{1 - v} \right) ,$$

$$\bar{v}_{2} = j + \frac{1}{2} \left( \frac{1}{1 - v_{*}} - \frac{1}{1 - v} \right) .$$
(48)

Moreover, using the jump conditions (39)<sub>3</sub> and (40)<sub>3</sub> together with (46) yields

$$T' = \frac{1}{2} (\delta_1 + \delta_0 - 1) + l_T + T_L ,$$
  
$$T'' = \frac{1}{2} (\delta_2 + \delta_1 - 1) + l_T + T_R .$$

Furthermore, using (47) in the above equations provides

$$T' = T_L + r(\mathbf{v}, \mathbf{v}_*) , \qquad (49)$$

$$T'' = T_R + r_*(v, v_*) , (50)$$

where

$$r(v, v_*) = \left\{ h - \frac{1}{2} \left( \frac{v_*}{1 + v_*} - \frac{v}{1 - v^2} \right) \right\} + l_T , \qquad (51)$$

$$r_{\star}(\mathsf{v},\mathsf{v}_{\star}) = \left\{ h - \frac{1}{2} \left( \frac{\mathsf{v}_{\star}}{1 - \mathsf{v}_{\star}^{2}} - \frac{\mathsf{v}}{1 - \mathsf{v}} \right) \right\} + l_{T} . \tag{52}$$

Notice that

$$r_*(-\mathsf{v}_*,-\mathsf{v})=r(\mathsf{v},\mathsf{v}_*)\ .$$

It is important to remark that a solution of the form (46) is not unique. In fact, equations (47)-(52) represent a two-parameter family of solutions where the phase boundary velocities v and  $v_*$  can be used as such parameters. The uniqueness issue is addressed in Section 6 with the postulation of a kinetic relation which singles out an appropriate pair  $(v, v_*)$  to fully determine the solution with two phase boundaries. A preliminary analysis regarding the existence of a solution is developed in the next section.

# 5.3 Phase segregation conditions and entropy inequality.

From (45) it is clear that for suitable initial data there exists a solution to the Riemann problem with no phase boundary. The solution which involves two phase boundaries requires further analysis. One has to ensure that the solution satisfies the entropy inequalities (39)<sub>4</sub> and (40)<sub>4</sub> and that  $(\delta_0, T_L) \in$ 

 $P_1, (\delta_1, T') \in P_3, (\delta_1, T'') \in P_3 \text{ and } (\delta_2, T_R) \in P_1, \text{ i.e.},$ 

$$\delta_{1} \geq \delta_{m}(T') ,$$

$$\delta_{1} \geq \delta_{m}(T'') ,$$

$$\delta_{0} \in (-1, \delta_{M}(T_{L})] ,$$

$$\delta_{2} \in (-1, \delta_{M}(T_{R})] ,$$

$$T' \in (0, T_{C}) ,$$

$$T'' \in (0, T_{C}) .$$
(53)

Conditions (53) are referred to as the *phase segregation* conditions. From (47), (49), (50), (51), and (28), it follows that the restrictions (53) and the entropy inequalities  $(39)_4$  and  $(40)_4$  are equivalent to

$$H_{0}(T_{L}, \mathsf{v}, \mathsf{v}_{*}) \leq (1 - \mathsf{m})h ,$$

$$H_{1}(T_{R}, \mathsf{v}, \mathsf{v}_{*}) \leq (1 - \mathsf{m})h ,$$

$$H_{2}(\mathsf{v}, \mathsf{v}_{*}) < h \leq H_{3}(T_{L}, \mathsf{v}, \mathsf{v}_{*}) ,$$

$$H_{4}(\mathsf{v}, \mathsf{v}_{*}) < h \leq H_{5}(T_{R}, \mathsf{v}, \mathsf{v}_{*}) ,$$

$$H_{6}(T_{L}, \mathsf{v}, \mathsf{v}_{*}) \leq h \leq H_{7}(T_{L}, \mathsf{v}, \mathsf{v}_{*}) ,$$

$$H_{8}(T_{R}, \mathsf{v}, \mathsf{v}_{*}) \leq h \leq H_{9}(T_{R}, \mathsf{v}, \mathsf{v}_{*}) ,$$

$$(54)$$

where the functions  $H_i$  are defined for  $-1 < v \le 0$ ,  $0 \le v_* < 1$  by

$$\begin{split} H_0(T_L,\mathsf{v},\mathsf{v}_\star) &= \delta_C + \mathsf{m}(T_L - T_C) - \frac{1}{2}(1-\mathsf{m}) \left\{ \frac{1}{1-\mathsf{v}} + \frac{1}{1+\mathsf{v}_\star} \right\} \\ &- \frac{\mathsf{m}}{2} \left\{ 1 + \frac{1}{1-\mathsf{v}^2} \right\} + \mathsf{m}l_T \;, \\ H_1(T_R,\mathsf{v},\mathsf{v}_\star) &= \delta_C + \mathsf{m}(T_R - T_C) - \frac{1}{2}(1-\mathsf{m}) \left\{ \frac{1}{1-\mathsf{v}} + \frac{1}{1+\mathsf{v}_\star} \right\} \\ &- \frac{\mathsf{m}}{2} \left\{ 1 + \frac{1}{1-\mathsf{v}_\star^2} \right\} + \mathsf{m}l_T \;, \\ H_2(\mathsf{v},\mathsf{v}_\star) &= \frac{1}{2} \left\{ \frac{1}{1+\mathsf{v}} - \frac{1}{1+\mathsf{v}_\star} \right\} - 1 \;, \\ H_3(T_L,\mathsf{v},\mathsf{v}_\star) &= \delta_C + 1 + \mathsf{M}(T_L - T_C) + H_2(\mathsf{v},\mathsf{v}_\star) \;, \\ H_4(\mathsf{v},\mathsf{v}_\star) &= \frac{1}{2} \left\{ \frac{1}{1-\mathsf{v}_\star} - \frac{1}{1-\mathsf{v}} \right\} - 1 \;, \\ H_5(T_R,\mathsf{v},\mathsf{v}_\star) &= \delta_C + 1 + \mathsf{M}(T_R - T_C) + H_4(\mathsf{v},\mathsf{v}_\star) \;, \\ H_6(T_L,\mathsf{v},\mathsf{v}_\star) &= \left\{ T_L \left( e^{\frac{l_T}{T_T}} - 1 \right) - l_T \right\} + \frac{1}{2} \left\{ \frac{\mathsf{v}_\star}{1+\mathsf{v}_\star} - \frac{\mathsf{v}}{1-\mathsf{v}^2} \right\} \;, \\ H_7(T_L,\mathsf{v},\mathsf{v}_\star) &= \left\{ (T_C - T_L) - l_T \right\} + \frac{1}{2} \left\{ \frac{\mathsf{v}_\star}{1+\mathsf{v}_\star} - \frac{\mathsf{v}}{1-\mathsf{v}^2} \right\} \;, \\ H_8(T_R,\mathsf{v},\mathsf{v}_\star) &= \left\{ (T_C - T_R) - l_T \right\} + \frac{1}{2} \left\{ \frac{\mathsf{v}_\star}{1-\mathsf{v}^2} - \frac{\mathsf{v}}{1-\mathsf{v}} \right\} \;. \end{split}$$

Notice the following symmetries:

$$\begin{split} H_2(\mathsf{v},\mathsf{v}_*) &= H_4(-\mathsf{v}_*,-\mathsf{v}) \;, \\ H_3(\cdot,\mathsf{v},\mathsf{v}_*) &= H_5(\cdot,-\mathsf{v}_*,-\mathsf{v}) \;, \\ H_6(\cdot,\mathsf{v},\mathsf{v}_*) &= H_8(\cdot,-\mathsf{v}_*,-\mathsf{v}) \;, \\ H_7(\cdot,\mathsf{v},\mathsf{v}_*) &= H_9(\cdot,-\mathsf{v}_*,-\mathsf{v}) \;. \end{split}$$

Equations  $(54)_{1,2,3,4}$  are equivalent to  $(53)_{1,2,3,4}$  respectively; the upper bounds in  $(54)_{5,6}$  are equivalent to the upper admissible value of the temperature in  $(53)_{5,6}$ , whereas the lower bounds in  $(54)_{5,6}$  are equivalent to the entropy inequalities  $(39)_4$  and  $(40)_4$  respectively. Notice that if the entropy inequalities are satisfied, then  $T' - T_L = r \ge 0$  at the phase boundary x/at = v and  $T'' - T_R = r_* \ge 0$  at the phase boundary  $x/at = v_*$ . Thus, necessarily, the conditions T' > 0 and T'' > 0 are satisfied.

The inequalities (54) determine, for fixed  $T_L$ ,  $T_R$ , a region in the  $(v, v_*, h)$ space where it is possible to have a two-parameter family of solutions of the
form (46). For simplicity, consider the case when  $l_T = 0$  which corresponds
to twinning. Furthermore, since it was assumed that  $\alpha = 0$ , then (30) and
(33) give

$$\mathsf{M} = -\mathsf{m} > 0 \;, \qquad \delta_C = \frac{1}{2} \;, \qquad \delta_C > \mathsf{M}T_C \;. \tag{55}$$

Under these assumptions, the functions  $H_1$  to  $H_9$  take the following form:

$$\begin{split} H_0(T_L,\mathsf{v},\mathsf{v}_*) &= \mathsf{M}(T_C - T_L) - \frac{1}{2}(1+\mathsf{M}) \left\{ \frac{1}{1-\mathsf{v}} + \frac{1}{1+\mathsf{v}_*} - 1 \right\} \\ &+ \frac{\mathsf{M}}{2} \left\{ \frac{1}{1-\mathsf{v}^2} \right\} \;, \\ H_1(T_R,\mathsf{v},\mathsf{v}_*) &= \mathsf{M}(T_C - T_R) - \frac{1}{2}(1+\mathsf{M}) \left\{ \frac{1}{1-\mathsf{v}} + \frac{1}{1+\mathsf{v}_*} - 1 \right\} \\ &+ \frac{\mathsf{M}}{2} \left\{ \frac{1}{1-\mathsf{v}_*^2} \right\} \;, \\ H_2(\mathsf{v},\mathsf{v}_*) &= \frac{1}{2} \left\{ \frac{1}{1+\mathsf{v}} - \frac{1}{1+\mathsf{v}_*} \right\} - 1 \;, \\ H_3(T_L,\mathsf{v},\mathsf{v}_*) &= \frac{3}{2} - \mathsf{M}(T_C - T_L) + H_2(\mathsf{v},\mathsf{v}_*) \;, \\ H_4(\mathsf{v},\mathsf{v}_*) &= \frac{1}{2} \left\{ \frac{1}{1-\mathsf{v}_*} - \frac{1}{1-\mathsf{v}} \right\} - 1 \;, \\ H_5(T_R,\mathsf{v},\mathsf{v}_*) &= \frac{3}{2} - \mathsf{M}(T_C - T_R) + H_4(\mathsf{v},\mathsf{v}_*) \;, \\ H_6(\mathsf{v},\mathsf{v}_*) &= H_2(\mathsf{v},\mathsf{v}_*) + \frac{3}{2} - \frac{1}{2} \left\{ \frac{1}{1-\mathsf{v}^2} \right\} \;, \\ H_7(T_L,\mathsf{v},\mathsf{v}_*) &= \{T_C - T_L\} + H_6(\mathsf{v},\mathsf{v}_*) \;, \\ H_8(\mathsf{v},\mathsf{v}_*) &= H_4(\mathsf{v},\mathsf{v}_*) + \frac{3}{2} - \frac{1}{2} \left\{ \frac{1}{1-\mathsf{v}_*^2} \right\} \;, \\ H_9(T_R,\mathsf{v},\mathsf{v}_*) &= \{T_C - T_R\} + H_8(\mathsf{v},\mathsf{v}_*) \;. \end{split}$$

Let

$$ar{H}_0 \equiv rac{H_0}{1+\mathsf{M}} \ , \quad ar{H}_1 \equiv rac{H_1}{1+\mathsf{M}} \ .$$

Notice that

$$H_6 > \bar{H}_0 \text{ if } v^2 > \frac{(\mathsf{M}T_C - 1/2) - \mathsf{M}T_L}{\mathsf{M}(T_C - T_L)}$$
.

But, from (55)3,  $(MT_C-1/2)-MT_L<0$ , hence  $H_6>\bar{H}_0$  for all v. A similar

analysis reveals that  $H_8 > \bar{H}_1$  for all  $v_*$ . Moreover, one has

$$H_2 > H_4 \text{ if } v_*^2 < v^2,$$
  
 $H_6 > H_8 \text{ if } v_*^2 < v^2,$   
 $H_2 > H_6 \text{ if } v^2 > c_1^2,$   
 $H_4 > H_8 \text{ if } v_*^2 > c_1^2,$ 

where

$$c_1^2 = \frac{2}{3} \ .$$

The lower bound for h is given by

for 
$$v^2 > v_*^2$$
  $H_{\min} = \begin{cases} H_6 & \text{for } 0 < v^2 < c_1^2 , \\ H_2 & \text{for } c_1^2 < v^2 < 1 , \end{cases}$ 

$$\text{for } v_*^2 > v^2 \quad H_{\min} = \begin{cases} H_8 & \text{for } 0 < v_*^2 < c_1^2 , \\ H_4 & \text{for } c_1^2 < v_*^2 < 1 . \end{cases}$$
(56)

Henceforth, for definiteness, it is assumed that

$$T_R > T_L (57)$$

For the upper bound, one has to consider two cases for the given initial temperatures  $T_L$  and  $T_R$ . Only the first case is considered here: Assume the given temperatures  $T_L$  and  $T_R$  satisfy

$$2(M+1)(T_R - T_L) < 1. (58)$$

Under this assumption, it follows that  $H_7 < H_3$  and  $H_9 < H_5$  for all  $v^2$  and  $v^2_*$ . Moreover,

$$H_{\text{max}} = \begin{cases} H_9 & \text{for } \mathbf{v}_*^2 < 1 - \frac{1}{4(T_R - T_L) + 1/(1 - \mathbf{v}^2)}, \\ H_7 & \text{for } \mathbf{v}_*^2 > 1 - \frac{1}{4(T_R - T_L) + 1/(1 - \mathbf{v}^2)}. \end{cases}$$
(59)

The lower and upper limits for h in the  $v^2, v_*^2$ -plane corresponding to the phase segregation conditions are shown in Figure 5. Notice that  $H_9 > H_8$  for any  $v^2, v_*^2$ , hence the admissible region is always non-empty. The values of  $v^2, v_*^2$  for which  $H_{\text{max}} \geq H_{\text{min}}$  correspond to the shaded region in Figure 6. Thus, the shaded region corresponds to the projection on the  $v^2, v_*^2$ -plane of the admissible region in the  $v^2, v_*^2$ , h-space. Typical cross sections of this region in the  $v^2, h$  and  $v_*^2, h$ -planes are shown at the end of next section in Figures 7 and 8.

# 6 Driving traction, kinetic relation and nucleation criterion.

As pointed out in Section 5.2, the solution involving two phase boundaries is not unique. The postulation of a kinetic relation at each phase boundary settles the uniqueness issue. In order to introduce the kinetic relation, the explicit form of the driving traction acting on each phase boundary is given below.

#### 6.1 Driving traction for phase boundaries.

For the thermoelastic material undergoing an adiabatic process, equation (26) at the phase boundary which has the high strain phase on its right becomes, with  $\alpha = 0$ ,

$$f = -\rho c \langle \theta \rangle \left\{ \log \frac{\theta^+}{\theta^-} - \frac{\lambda_T}{c\theta_T} \right\} . \tag{60}$$

If the high strain phase is on the *left* of the phase boundary, then (26) becomes

$$f = \rho c \langle \theta \rangle \left\{ \log \frac{\theta^-}{\theta^+} - \frac{\lambda_T}{c\theta_T} \right\} . \tag{61}$$

Consider a dimensionless driving traction defined as

$$f \equiv \frac{f}{\mu \gamma_T^2} \ . \tag{62}$$

From (33), (60), (61), (49) and (50), the driving traction at the phase boundary  $x/at = \mathbf{v}$  is

$$f = -F \left[ T_L, r(\mathsf{v}, \mathsf{v}_*) \right] , \qquad (63)$$

and the driving traction at the phase boundary  $x/at = \mathsf{v}_*$  is

$$f_* = F[T_R, r_*(v, v_*)],$$
 (64)

where

$$F(T,r) = \left(T + \frac{r}{2}\right) \left\{ \log\left(1 + \frac{r}{T}\right) - \frac{l_T}{T_T} \right\} , \qquad (65)$$

and  $r, r_*$  are given by (51)-(52). In the purely mechanical case, ABEYARATNE & KNOWLES [2] showed that, under certain assumptions, the corresponding Riemann problem was symmetric in the sense that  $v = -v_*$  and  $f = -f_*$  so that the problem reduces to a one-parameter family of solutions. The adiabatic Riemann problem does not exhibit such symmetry. One has to consider, separately, a kinetic relation for each propagating phase boundary. Nevertheless, one can easily check that the solution is symmetric when  $T_L = T_R$ .

#### 6.2 Kinetic relations.

From (19), (21), (22) and (23), the dimensionless rate of entropy production for a segment of the bar containing a phase boundary during some time interval can be expressed by

$$\bar{\Gamma} \equiv \frac{1}{\rho ac} \Gamma = \frac{\mathsf{fv}}{\langle T \rangle} \ . \tag{66}$$

If, following [1] and [3], the quantity  $f/\langle T \rangle$  is identified as an affinity and v as the corresponding flux, then the kinetic relation relates the affinity to the flux and, in this case, to the temperature on one side of the phase boundary. The temperature is not considered as an affinity (it describes the state of the material). Therefore, the relation between the affinity and the flux is of the

form

$$\frac{\mathsf{f}}{\langle T \rangle} = \varphi_{ij}(T,\mathsf{v}) \ ,$$

where the subscripts refer to the low and high strain phases  $P_1$  and  $P_3$ . Thus,

$$\frac{\mathsf{f}}{T_L + r/2} = \varphi_{13}(T_L, \mathsf{v}) , \qquad (67)$$

$$\frac{f_*}{T_R + r_*/2} = \varphi_{31}(T_R, \mathsf{v}_*) \ . \tag{68}$$

Clearly, it is required that

$$\varphi_{13}(\cdot, \mathbf{v}) = -\varphi_{31}(\cdot, -\mathbf{v}) . \tag{69}$$

The kinetic relation has to satisfy some restrictions that arise upon enforcement of the entropy inequality. Since  $\bar{\Gamma}$  is non-negative, then  $\varphi_{ij}$  must be such that

$$\varphi_{ij}(T, \mathbf{v})\mathbf{v} \geq 0$$
 .

This implies that if  $\varphi_{ij}$  is differentiable with respect to v, then

$$\varphi_{ij}(T,0) = 0 , \quad \frac{\partial \varphi_{ij}}{\partial \mathbf{v}}(T,0) \ge 0 .$$
(70)

Furthermore, assume that  $\varphi_{ij}$  is strictly monotonically increasing with v.

Returning to the special case where  $l_T = 0$ , from (67), (68), (69), (63), (64) and (65), one has

$$\log\left(1+\frac{r}{T_L}\right) = \varphi_{31}(T_L, -\mathsf{v}) \;, \quad \log\left(1+\frac{r_*}{T_R}\right) = \varphi_{31}(T_R, \mathsf{v}_*) \;;$$

therefore,

$$r = T_L \left( e^{\varphi_{31}(T_L, -\mathbf{v})} - 1 \right) , \quad r_* = T_R \left( e^{\varphi_{31}(T_R, \mathbf{v}_*)} - 1 \right) .$$

Using (51) and (52) with  $l_T = 0$  provides

$$h + \frac{1}{2} \left( \frac{\mathsf{v}}{1 - \mathsf{v}^2} - \frac{\mathsf{v}_*}{1 + \mathsf{v}_*} \right) = T_L \left( e^{\varphi_{31}(T_L, -\mathsf{v})} - 1 \right) , \tag{71}$$

$$h + \frac{1}{2} \left( -\frac{\mathsf{v}_*}{1 - \mathsf{v}_*^2} + \frac{\mathsf{v}}{1 - \mathsf{v}} \right) = T_R \left( e^{\varphi_{31}(T_R, \mathsf{v}_*)} - 1 \right) . \tag{72}$$

Consider the restriction of the function  $\varphi_{31}(T,\cdot)$  to non-negative values of its argument. Define

$$\tilde{\varphi}_{31}(T, \mathsf{v}^2) \equiv \varphi_{31}(T, \mathsf{v}) \qquad \text{for } \mathsf{v} \ge 0 \ . \tag{73}$$

Recall that the phase velocities are -v > 0 and  $v_* > 0$ , hence, subtracting (72) from (71) and using (73) gives

$$\frac{\mathbf{v}_{*}^{2}}{1 - \mathbf{v}_{*}^{2}} + 2T_{R} \left( e^{\tilde{\varphi}_{31}(T_{R}, \mathbf{v}_{*}^{2})} - 1 \right) = \frac{\mathbf{v}^{2}}{1 - \mathbf{v}^{2}} + 2T_{L} \left( e^{\tilde{\varphi}_{31}(T_{L}, \mathbf{v}^{2})} - 1 \right) . \tag{74}$$

From the properties of the kinetic relation  $\varphi_{31}$ , the function  $\tilde{\varphi}_{31}$  increases monotonically with  $v^2$ . As a function of  $v^2$ , (resp.  $v_*^2$ ), the left-hand side (right-hand side) of (74) is strictly monotonically increasing from 0 at  $v^2 = 0$  ( $v_*^2 = 0$ ) to  $+\infty$  at  $v^2 = 1$  ( $v_*^2 = 1$ ). Thus, there is a unique  $v_*^2 \in [0,1)$  for a given  $v^2 \in [0,1)$ . Therefore, it is possible to define a functional relation

between  $v_*^2$  and  $v^2$ , say

$$v^2 = \Phi(v_*^2, T_L, T_R) \ . \tag{75}$$

Notice that, since  $\mathbf{v} < 0$ , then  $\mathbf{v} = -\sqrt{\Phi(\mathbf{v}_*^2, T_L, T_R)}$ . Henceforth, let

$$\begin{split} V &= \sqrt{\Phi(\mathsf{v}_*^2, T_L, T_R)} \ , \\ \varphi_L &= \tilde{\varphi}_{31}(T_L, \mathsf{v}^2) = \tilde{\varphi}_{31}(T_L, \Phi(\mathsf{v}_*^2, T_L, T_R)) \ , \\ \varphi_R &= \tilde{\varphi}_{31}(T_R, \mathsf{v}_*^2) \ . \end{split}$$

Adding (71) and (72) and using (73), (75) and the above notation, one has

$$h = \Psi(\mathbf{v}_{*}^{2}, T_{L}, T_{R})$$

$$= \frac{T_{L}}{2} \left( e^{\varphi_{L}} - 1 \right) + \frac{T_{R}}{2} \left( e^{\varphi_{R}} - 1 \right) + \frac{1}{2} \left\{ \frac{2\mathbf{v}_{*} - \mathbf{v}_{*}^{2}}{1 - \mathbf{v}_{*}^{2}} + \frac{2V - V^{2}}{1 - V^{2}} \right\} . \tag{76}$$

The function  $\Psi$  is strictly monotonically increasing in  $\mathbf{v}_*^2$  from 0 at  $\mathbf{v}_*^2 = 0$  to  $+\infty$  at  $\mathbf{v}_*^2 = 1$ . Therefore, for a given h in the admissible range, (76) singles out a unique  $\mathbf{v}_*^2$  which, by (75), provides a unique  $\mathbf{v}^2$ . This fully determines a unique solution of the form (46).

The fact that a solution exists can be seen by the following analysis. The

lower bounds  $H_6$  and  $H_8$  of the admissible region can be expressed as

$$\begin{split} \tilde{H}_6(\mathbf{v}_*^2, T_L, T_R) &= H_6(\Phi(\mathbf{v}_*^2, T_L, T_R), \mathbf{v}_*^2) \\ &= \frac{1}{2} \left\{ \frac{1 + V - V^2}{1 - V^2} - \frac{1}{1 + \mathbf{v}_*} \right\} \;, \\ \tilde{H}_8(\mathbf{v}_*^2, T_L, T_R) &= H_8(\Phi(\mathbf{v}_*^2, T_L, T_R), \mathbf{v}_*^2) \\ &= \frac{1}{2} \left\{ \frac{1 + \mathbf{v}_* - \mathbf{v}_*^2}{1 - \mathbf{v}_*^2} - \frac{1}{1 + V} \right\} \;. \end{split}$$

Notice that  $\Psi(\mathsf{v}_*, T_L, T_R) \geq \max_{\mathsf{v}_*^2} [\tilde{H}_6(\mathsf{v}_*^2, T_L, T_R), \tilde{H}_8(\mathsf{v}_*^2, T_L, T_R)]$ . Moreover, the upper bound  $H_9$  is such that  $H_9 = (T_C - T_R)$  for  $\mathsf{v}_* = \mathsf{v} = 0$ . Hence, by continuity, there exists a range of values of h in the admissible region for which  $\max[H_6, H_8] \leq h = \Psi < H_9$ , thus the *existence* of a solution of the form (46) is guaranteed. A complete analysis of solvability requires further knowledge of a specific kinetic relation.

#### 6.3 Nucleation criterion.

As shown in Sections 5.1 and 5.2, there are two different kinds of solutions for the adiabatic Riemann problem. One can interpret the no-phase boundary solution as the limit of the two-phase boundary solution when  $\mathbf{v} \to 0^-$  and  $\mathbf{v}_* \to 0^+$ . Now, if the initial datum satisfies (45), it is possible to have a solution with no phase boundaries of the form (42). Assuming that  $T_R > T_L$ and using (55)<sub>1</sub>, then (44) becomes

$$-1 < h \le \frac{1}{2} - \mathsf{M}(T_C - T_L) \ . \tag{77}$$

On the other hand, the lower bound for h corresponding to the solution with two phase boundaries at  $v^2 = v_*^2 = 0$  is  $H_{\min}(0,0) = 0$  and the upper bound is  $H_{\max}(0,0) = (T_C - T_R)$ . Moreover, the curve defined by (76) passes through the origin, hence, if

$$\frac{1}{2} - \mathsf{M}(T_C - T_L) < (T_C - T_R)$$

then there exists an overlapping range for the initial datum h for which it is possible to have either kind of solution:

if 
$$\begin{cases} -1 < h \le 0 \\ 0 < h \le \frac{1}{2} - \mathsf{M}(T_C - T_L) \end{cases}$$
 then 
$$\begin{cases} \text{No phase change solution.} \\ \text{Both types of solutions.} \end{cases}$$
 (78)

To select the appropriate solution, a nucleation criterion is required. Following [2], assume there is a critical value  $f_{cr}(T)$  of the driving traction at which a transformation from low to high strain phase occurs. In this case, the critical value depends on the temperature of the corresponding low strain phase temperature. From (51), (52), (63), (64) and (65), nucleation occurs when

$$|\mathsf{f}| = F(T_L, r(h, \mathsf{v}, \mathsf{v}_*)) = \mathsf{f}_{\mathrm{cr}}(T_L) \tag{79}$$

for the leftward moving phase boundary and

$$f_* = F(T_R, r_*(h, v, v_*)) = f_{cr}(T_R)$$
 (80)

for the rightward moving phase boundary. Although h is considered as fixed (initial conditions), the explicit dependence of r and  $r_*$  on h is shown for clarity. Equations (79) and (80) define two surfaces on the  $\mathsf{v}^2, \mathsf{v}^2_*, h$ -space. The intersection of the region where  $\mathsf{f} \geq \mathsf{f}_{\mathsf{cr}}(T_L)$  and  $|\mathsf{f}_*| \geq \mathsf{f}_{\mathsf{cr}}(T_R)$  corresponds to the region where nucleation occurs. Typical cross sections of this region are shown by the shaded area in Figures 7 and 8.

# 7 Nucleation: nontrivial solution for uniform data.

The importance of the Riemann problem with uniform initial data is related to its connection with the nucleation criterion. Since the bar is initially in the same phase and there are no discontinuities, the existence of a nontrivial solution (where two phase boundaries nucleate from an arbitrary point) could, in principle, provide a restriction on the critical value of the driving traction  $f_{cr}$ . Suppose that the initial data of the Riemann problem of Section 5.2 is such that  $\delta_L = \delta_R = \delta_*$  and  $T_L = T_R = T_*$ . Since the system of equations (34)-(36) and the jump conditions (38)-(40) are homogeneous, then the problem admits a trivial solution  $\delta(x,t) = \delta_*$  and  $T(x,t) = T_* \forall x,t$ . Nevertheless, there is also a nontrivial solution. Since  $T_L = T_R$  and in view of the properties of the kinetic relation  $\varphi_{ij}$ , equation (74) implies that

$$\mathsf{v}^2 = \mathsf{v}_*^2 \quad \Rightarrow \quad \mathsf{v} = -\mathsf{v}_* \ .$$

From (47)-(52), there exists a one-parameter family of nontrivial solutions for the Riemann problem with uniform initial data of the following form (parametrized by  $v_*$ ):

$$\delta(x,t) = \begin{cases} \delta_{*} & -\infty < x < -at ,\\ \delta_{0} & -at < x < -av_{*}t ,\\ \delta_{1} & -av_{*}t < x < av_{*}t ,\\ \delta_{0} & av_{*}t < x < at ,\\ \delta_{*} & at < x < \infty , \end{cases}$$
(81)

and

$$T(x,t) = \begin{cases} T_* & -\infty < x < -av_*t ,\\ T' & -av_*t < x < av_*t ,\\ T_* & av_*t < x < \infty , \end{cases}$$
 (82)

where

$$\begin{split} \delta_0 &= \delta_* - \left(\frac{\mathsf{v}_*}{1 - \mathsf{v}_*^2}\right) \;\;, \\ \delta_1 &= \delta_* + \left(\frac{1}{1 + \mathsf{v}_*}\right) \;\;, \\ T' &= \delta_* - \frac{1}{2} \left(\frac{2\mathsf{v}_* - \mathsf{v}_*^2}{1 - \mathsf{v}_*^2}\right) + T_* \;\;. \end{split}$$

Notice that, in view of the analysis of Section 6.2, a solution of the form (81), (82) exists. Using the notation of Section 6.2, it follows that  $V = v_*$  and

 $\varphi_L = \varphi_R = \varphi_* = \tilde{\varphi}(T_*, \mathsf{v}_*^2)$ . Equation (76), together with (43), becomes

$$h = \delta_* = T_* \left( e^{\varphi_*} - 1 \right) + \left\{ \frac{2\mathsf{v}_* - \mathsf{v}_*^2}{1 - \mathsf{v}_*^2} \right\} .$$

The nucleation criterion was introduced in terms of the driving traction which, in this case, can be written as

$$f(T_*, r(\delta_*, \mathsf{v}_*)) = \left(T_* + \frac{r(\delta_*, \mathsf{v}_*)}{2}\right) \left[\log\left(1 + \frac{r(\delta_*, \mathsf{v}_*)}{T_*}\right)\right] ,$$

where

$$r(\delta_*, \mathsf{v}_*) = \delta_* - \frac{1}{2} \left[ \frac{2\mathsf{v}_* - \mathsf{v}_*^2}{1 - \mathsf{v}_*^2} \right] .$$

In order to have an admissible solution, the phase segregation conditions and entropy inequality requirements have to be enforced. From Section 5.3, the lower bound for the value of h is given by

$$H_{\min} = \begin{cases} \tilde{H}_6 = \tilde{H}_8 = \frac{1}{2} \left( \frac{2 \mathsf{v}_* - \mathsf{v}_*^2}{1 - \mathsf{v}_*^2} \right) & 0 < \mathsf{v}_*^2 < c_1^2 \ , \\ \tilde{H}_2 = \tilde{H}_4 = \frac{\mathsf{v}_*}{1 - \mathsf{v}_*^2} - 1 & c_1^2 < \mathsf{v}_*^2 < 1 \ . \end{cases}$$

Recall that the functions  $\tilde{H}_6$  and  $\tilde{H}_8$  are related to the entropy inequality  $(39)_4$  and  $(40)_4$ , whereas the functions  $\tilde{H}_2$  and  $\tilde{H}_4$  represent the restriction  $T' = T'' < T_C$ . The upper bound for the admissible region is given by

$$H_{\text{max}} = H_7 = H_9 = \frac{1}{2} \left( \frac{2\mathsf{v}_* - \mathsf{v}_*^2}{1 - \mathsf{v}_*^2} \right) \ .$$

The admissible region is shown in Figure 9. From this, one can see that there is a minimum value for  $\delta_*$  below which no nucleation occurs (in this case,

 $\delta_*=0$  at  $v_*^2=0$ ). Observe that this lower bound is given by the entropy inequality (it corresponds to f=0). This analysis confirms the fact that nucleation occurs at a critical value such that  $f_{cr}v_*\geq 0$  (as required by the entropy inequality) but fails to restrict the nucleation criterion in any other way.

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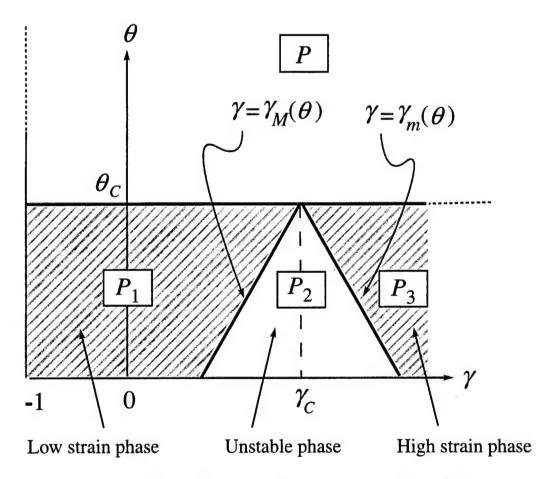


Figure 1: Material phases in the temperature-strain plane.

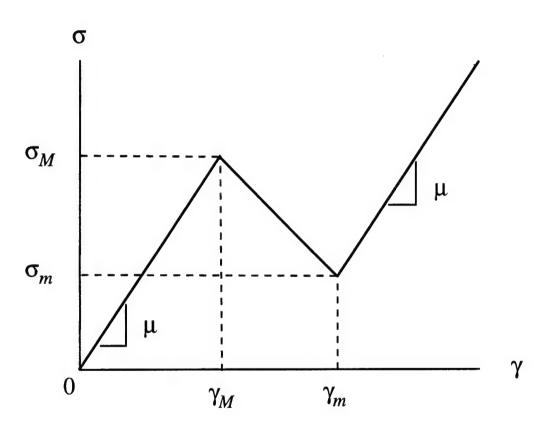


Figure 2: Stress-strain relation for  $\alpha = 0$ .

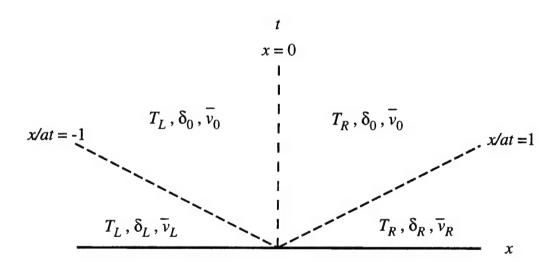


Figure 3: Solution with no phase boundary.

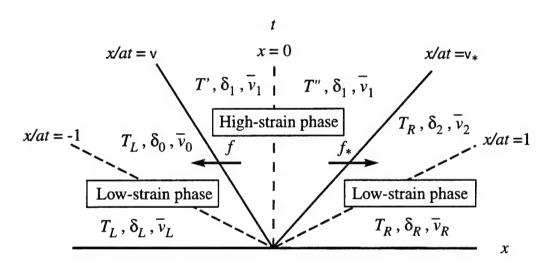


Figure 4: Solution with two phase boundaries.

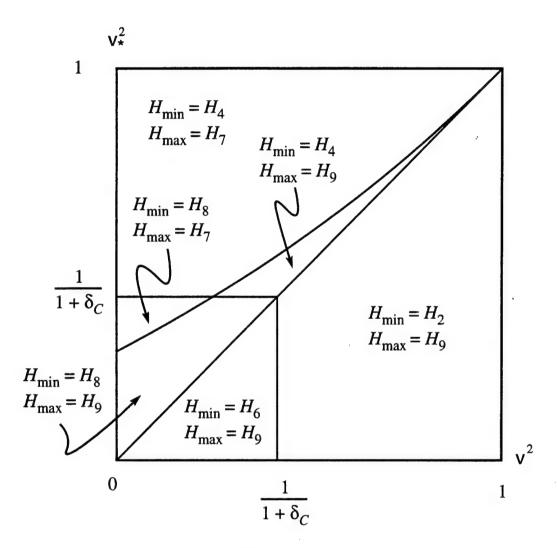


Figure 5: Lower and upper admissible limits for the initial datum h on the  $\mathbf{v}^2, \mathbf{v}_*^2$ -plane.

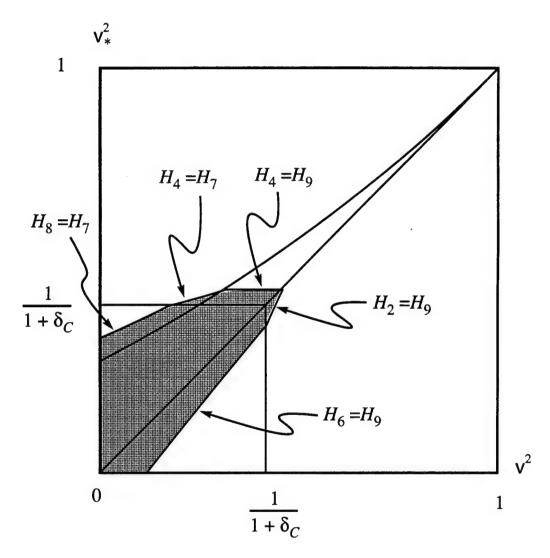


Figure 6: Projection of the admissible region from the  $v^2, v_*^2, h$ -space onto the  $v^2, v_*^2$ -plane.

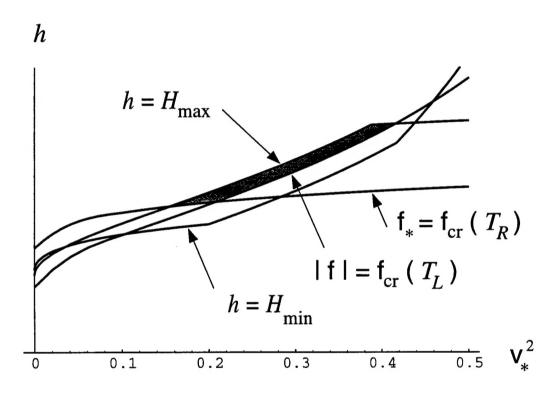


Figure 7: Admissible values of the inital datum h on the plane  $v^2 = 0.2$ .

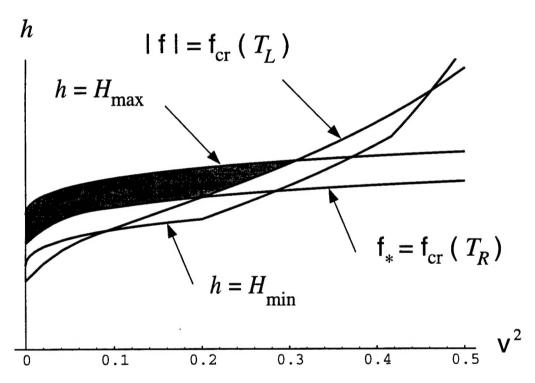


Figure 8: Admissible values of the inital datum h on the plane  $v_*^2 = 0.2$ .

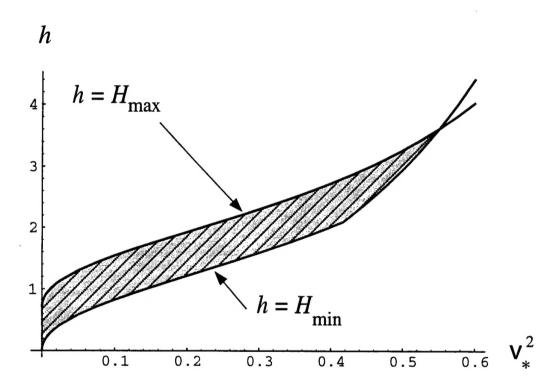


Figure 9: Admissible region for uniform data problem.

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The dynamical aspects of solid-solid phase transformations are studied within the framework of the theory of thermoelasticity. A problem of the Riemann type for a one-dimensional bar undergoing an adiabatic process is analyzed. It is shown that by imposing a kinetic relation and a nucleation criterion it is possible to single out a unique solution. This extends to the thermomechanical case results previously found in a purely mechanical context.						
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